THE MERCK INDEX

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TWELFTH EDITION

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Published by
Merck Research Laboratories
Division of
MERCK & CO., INC.
Whitehouse Station, NJ

1996

MERCK & CO., INC.
Whitehouse Station, N.J.
U.S.A.

1st Edition—1889
2nd Edition—1896
3rd Edition—1907
4th Edition—1930
5th Edition—1940
6th Edition—1952
7th Edition—1960
8th Edition—1968
9th Edition—1976
10th Edition—1983
11th Edition—1989

Library of Congress Catalog
Card Number 89-60001
ISBN Number 0911910-12-3

First Printing—March 1996
Second Printing—April 1997

H_2SO_4: Kamm, Marvel, *Org. Syn.* coll. vol. I, 29 (1941). By phosphorus and bromine method: Goshorn *et al., ibid.* 36. Absorption spectrum: Hantzsch, *Ber.* 58, 619 (1925). Physical properties: Mumford, Phillips, *J. Chem. Soc.* 1950, 75. Toxicity data: E. H. Vernot *et al., Toxicol. Appl. Pharmacol.* 42, 417 (1977).

Colorless, flammable, volatile liq; ethereal odor; burning taste; becomes yellowish on exposure to air and light. Vapor harmful. d_4^{20} 1.4612; d_4^{25} 1.4515. bp 38.2°. mp −119°. n_D^{20} 1.4242. Soly in water (g/100 g) at 0°: 1.067; 10°: 0.965; 20°: 0.914; 30°: 0.896; miscible with alcohol, ether, chloroform and with other organic solvents. Explosive limits (% by vol in air), lower 6.75, upper 11.25. Autoignition temp 952°F (511°C). LC_{50} rats, mice (ppm): 27000, 16200 (Vernot).

Caution: Potential symptoms of overexposure are irritation of eyes, respiratory system and skin; central nervous system depression; pulmonary edema; liver and kidney disease; cardiac arrhythmias; cardiac arrest. *See NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 90-117, 1990) p 106.

USE: Ethylating agent in organic synthesis; as refrigerant. Formerly used as a topical and inhalation anesthetic.

3820. Ethyl α-Bromopropionate. *2-Bromopropanoic acid ethyl ester.* $C_5H_9BrO_2$; mol wt 181.03. C 33.17%, H 5.01%, Br 44.14%, O 17.68%. $CH_3CHBrCOOC_2H_5$.

Liquid; sharp, pungent odor; becomes yellow on exposure to light. d_{20}^{20} 1.447. bp 159-160°; also stated as 160-165°. n_D^{20} 1.4469. Insol in water; miscible with alcohol, ether. *Protect from light.*

3821. Ethyl *tert*-Butyl Ether. *2-Ethoxy-2-methylpropane; tert-butyl ethyl ether;* ethyl *tert*-butyl oxide; 1,1-dimethylethyl ethyl ether; ethyl 1,1-dimethylethyl ether; ETBE. $C_6H_{14}O$; mol wt 102.18. C 70.53%, H 13.81%, O 15.66%. $(CH_3)_3C(OCH_3CH_3)$. Prepn J. U. Nef, *Ann.* 309, 126 (1899). Synthesis: J. F. Norris, G. W. Rigby, *J. Am. Chem. Soc.* 54, 2088 (1932). Physical properties: T. W. Evans, K. R. Edlund, *Ind. Eng. Chem.* 28, 1186 (1936). Thermal decomposition: N. J. Daly, C. Wentrup, *Aust. J. Chem.* 21, 1535 (1968). Brief review focusing on use as gasoline additive: M. Iborra *et al., Chemtech.* 18, 120 (1988).

bp 69-71°. fp −94.0°. Also reported as bp 73.1° (Norris, Rigby). d_0^{25} 0.7364. n_D^{25} 1.3728. Also reported as bp 72.8°, (Evans, Edlund). d_4^{15} 0.7456; d_4^{20} 0.7404; d_4^{25} 0.7353, d_4^{30} 0.7300. n_D^{20} 1.3760. Vapor pressure at 25°: 130 mm Hg. Heat vaporization: 74.3 cal/g. Specific heat (liquid) at 25°: 0.51 cal/g/°C. Surface tension at 24°: 19.8 dynes/cm. Soly in water (20°): 1.2 g/100 g soln. Soly of water in compound (20°): 0.5 g/100 g soln.

USE: Gasoline additive.

3822. Ethyl Butyrate. *Butanoic acid ethyl ester; butyric acid ethyl ester;* ethyl *n*-butyrate. $C_6H_{12}O_2$; mol wt 116.16. C 62.04%, H 10.41%, O 27.55%. $CH_3CH_2CH_2COOC_2H_5$. Toxicity data: P. M. Jenner *et al., Food Cosmet. Toxicol.* 2, 327 (1964).

Colorless liq; pineapple odor. d_4^{20} 0.879. bp 120-121°. mp −93°. n_D^{20} 1.400. Flash pt, closed cup: 78°F (25°C); open cup: 85°F (29°C). Sol in about 150 parts water; misc with alcohol, ether. LD_{50} orally in rats: 13,050 mg/kg (Jenner).

USE: Manuf artificial rum; perfumery; the alcoholic soln constitutes the so-called *"pineapple oil"*.

3823. Ethyl Caprate. *Decanoic acid ethyl ester;* ethyl decanoate. $C_{12}H_{24}O_2$; mol wt 200.32. C 71.95%, H 12.08%, O 15.97%. $CH_3(CH_2)_8COOC_2H_5$.

Colorless liq. d^{20} 0.862. bp 243-245°. Insoluble in water; miscible with alcohol, chloroform, ether.

USE: Manuf wine bouquets, cognac essence.

3824. Ethyl Caproate. *Hexanoic acid ethyl ester;* ethyl hexanoate. $C_8H_{16}O_2$; mol wt 144.21. C 66.63%, H 11.18%, O 22.19%. $CH_3(CH_2)_4COOC_2H_5$.

Colorless to yellowish liquid; pleasant odor. d^{20} 0.87[illegible]. bp 166-167°. Insol in water; miscible with alcohol, ether

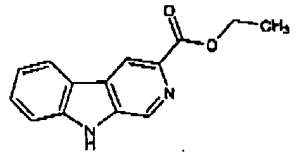
USE: Manuf artificial fruit flavors.

3825. Ethyl Caprylate. *Octanoic acid ethyl ester;* ethyl octanoate; ethyl octylate: $C_{10}H_{20}O_2$; mol wt 172.27. C 69.72%, H 11.70%, O 18.58%. $CH_3(CH_2)_6COOC_2H_5$.

Colorless, clear, very mobile liquid; pleasant, pineapple odor. d^{17} 0.878. bp 207-209°. Insol in water; misc with alcohol, ether. LD_{50} orally in rats: 25,960 mg/kg. P. M. Jenner *et al., Food Cosmet. Toxicol.* 2, 327 (1964).

USE: Manuf fruit ethers; constit of enanthic, coccic, and cognac ethers.

3826. Ethyl β-Carboline-3-carboxylate. *9H-Pyrido[3,4-b]indole-3-carboxylic acid ethyl ester;* ethyl norharmancarboxylate; β-CCE. $C_{14}H_{12}N_2O_2$; mol wt 240.26. C 69.99%, H 5.03%, N 11.66%, O 13.32%. Deriv of *β-carboline* that is a potent displacer of ^{3}H-diazepam from brain benzodiazepine receptors. Isoln from human urine and brain and binding site study: C. Braestrup *et al., Proc. Nat. Acad. Sci. USA* 77, 2288 (1980). Initially thought to be an endogenous ligand for benzodiazepine receptors in mammalian CNS, it is now believed to be formed during isoln and extraction procedures, R. F. Squires in *GABA and Benzodiazepine Receptors,* E. Costa *et al.,* Eds. (Raven Press, New York, 1980) pp 129-138; M. Nielson *et al., J. Neurochem.* 36, 276 (1981). Synthesis and psychotropic activity: Japan. Kokai 81 43283 (to Schering AG), *C.A.* 95, 115508a (1981); U. Eder *et al.,* Eur. pat. Appl. 30,254 (1981 to A/S Perrosan; Schering AG). β-CCE has been shown to lower seizure threshold and to reverse the sedative effect of flurazepam, q.v.: P. J. Cowen *et al., Nature* 290, 54 (1981). Neurochemical and pharmacological actions of β-CCE and other β-carbolines: M. Cain *et al., J. Med. Chem.* 25, 1081 (1982). Anxiogenic and convulsant properties: L. Prado de Carvalho *et al., Nature* 301, 64 (1983).



mp 229-233°. uv max (pH 7): 215, 242, 279 nm.

3-Hydroxymethyl-β-carboline, $C_{12}H_{10}N_2O$, *9H-pyrido[3,4-b]indole-3-methanol, 3-HMC.* Prepn: F. Hamaguchi, S. Ohki, *Heterocycles* 8, 383 (1977); M. Cain *et al., loc. cit.* Antagonism of anticonvulsant and anxiolytic actions of diazepam: P. Skolnick *et al., Eur. J. Pharmacol.* 68, 381 (1980). Crystals, mp 225-228°.

USE: As tools for studying benzodiazepine receptors.

3827. Ethyl Carbonate. *Carbonic acid diethyl ester;* diethyl carbonate; Eufin. $C_5H_{10}O_3$; mol wt 118.13. C 50.84%, H 8.53%, O 40.63%. $(C_2H_5O)_2C{=}O$. Prepn: Palomaa *et al., Ber.* 72, 313 (1939). Manuf: Mador, Blackham, U.S. pat. 3,114,762 (1963 to Natl. Distillers & Chem.).

Liquid, bp 126°. Pleasant ethereal odor, mp −43°. Flash pt, closed cup: 77°F (25°C). d_4^{20} 0.9764. n_D^{20} 1.3843. Practically insol in water; miscible with alcohol, ether.

USE: Solvent for nitrocellulose; manuf radio tubes; fixing rare earths to cathode elements.

3828. Ethyl Cellulose. *Cellulose ethyl ether;* Ethocel. Prepd from wood pulp or chemical cotton by treatment with alkali and ethylation of the alkali cellulose with ethyl chloride. Review and bibliography: E. Ott, *Cellulose and Cellulose Derivatives* (New York, 2nd ed., 1955).

White granules. Soly is dependent upon the degree of substitution. Commercial ethyl cellulose has an ethoxy content of 43-50%. A 47% product softens at 140° and is sol in ethyl acetate, ethylene dichloride, benzene, toluene, xylene, butyl acetate, acetone, methanol, ethanol, butanol, carbon tetrachloride. To avoid brittleness, ethyl cellulose formulations usually include an antioxidant such as hydroquinone monobenzyl ether, 4-hexylpyrocatechol, or diphenylamine.

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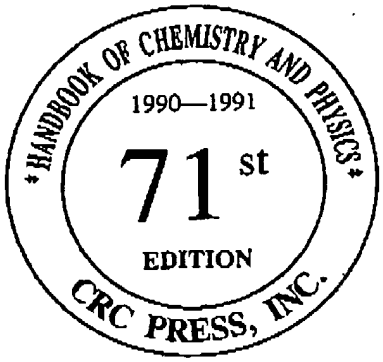

Editor-in-Chief,

David R. Lide, Ph.D.

CRC Press
Boca Raton Ann Arbor Boston

PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS (Continued)

No.	Name, Synonyms, and Formula	Mol. wt.	Color, crystalline form, specific rotation and [θ] (log ε)	b.p. °C.	m.p. °C	Density	n_D	Solubility	Ref.
4830	Cellulose, hexanitrate or Gun cotton $(C_{12}H_{14}N_6O_{16})_x$	(594.27)$_x$	wh amor	.....	160-70 (ign)	1.66	.....	pn NO_3	.....
4831	Cellulose, pentanitrate $(C_{12}H_{15}N_5O_{15})_x$	(549.28)$_x$	wh amor	.....	1.66	.....	.....	eth-al	.....
4832	Cellulose, tetranitrate or in Collodion $(C_{12}H_{16}N_4O_{14})_x$	(504.28)$_x$	wh amor	.....	.....	1.66	.....	eth-al	.....
4833	Cellulose, triacetate $(C_{12}H_{16}O_8)_x$	(288.25)$_x$	yesh fl $[\alpha]_D$ −22.5 (chl)	.....	.....	.....	.....	aa	.....
4834	Cellulose, triethylether or Ethylcellulose $(C_{12}H_{23}O_5)_x$	(246.30)$_x$	wh nd (bz) $[\alpha]^{30}_D$ + 26.1 (bz)	.....	240-55	.....	.....	eth	.....
4835	Cellulose, trinitrate or in Collodion $(C_6H_7N_3O_{11})_x$	(459.28)$_x$	wh	.....	.....	1.66	.....	ace, aa	.....
4836	Cepharanthine $C_{37}H_{38}N_2O_6$	606.72	ye amor pw $[\alpha]^{20}_D$ + 277 (chl)	.....	145-55	.....	.....	al, eth, ace, bz	C49, 1745
4837	Cerene or Isohexacosane $CH_3(CH_2)_{24}CH_3$	366.71	pl (eth), sc (w)	207[17]	61	.....	.....	al, eth	B1[3], 143
4838	Cerulignone $[(C_6H_2O(CH_3O)_2)_2]$	304.30	bl gr	.....	.....	.....	.....	.....	B8[1], 573
4839	Cetane or Hexadecane $CH_3(CH_2)_{14}CH_3$	226.45	lf (ace)	287, 149[19]	18.2	0.7733[20/4]	1.4345	eth	B1[1], 537
4840	Cetene or 1-Hexadecene $CH_3(CH_2)_{13}CH{=}CH_2$	224.43	lf	284.4, 155[15]	4.1	0.7811[20/4]	1.4412[20]	al, eth, peth	B1[1], 927
4841	Cetyl alcohol or 1-Hexadecanol $CH_3(CH_2)_{15}CH_2OH$	242.45	fl (AcOEt)	344, 190[15]	50	0.8176[50/4]	1.4283[50]	eth, ace, bz, chl	B1[1], 1876
4841	Cetylamine or 1-Amino hexadecane $CH_3(CH_2)_{14}CH_2NH_2$	241.46	lf	323.5, 144[5]	46.8	0.8129[50/4]	1.4496[50]	al, eth, ace, bz, chl	B4[1], 818
4842	Cetylamine or 1-Amino hexadecane $CH_3(CH_2)_{14}CH_2NH_2$	241.46	lf	323.5, 144[5]	46.8	0.8129[50/4]	1.4496[50]	al, eth, ace, bz, chl	B4[1], 818
4843	Cetyl Phenyl Ether or Hexadecyl phenyl ether $C_{16}H_{33}OC_6H_5$	318.54	lf (al)	200[1]	41.8	0.8434[41]	1.4556[25]	.....	B6[3], 555
4844	Cetyl sulfate $[C_{16}H_{33}O]_2SO_2$	546.93	.....	.....	66.2	.....	.....	w	B1[1], 1879
4845	Cevagenine $C_{27}H_{43}NO_3$	509.64	nd (MeOH-eth), $[\alpha]^{20/D}$ −47.5 (al)	.....	246-8	.....	.....	.....	B21[1], 6815
4846	Chalcone dibromide-*(threo)* $C_6H_5CHBrCHBrCOC_6H_5$	368.07	nd (al)	.....	122-3	.....	.....	al	B7[2], 2155
4847	Chalcone dibromide-*(erythro)* $C_6H_5CHBrCHBrCOC_6H_5$	368.07	pr or nd (al)	.....	159-60	.....	.....	.....	B7[2], 2154
4848	Chalcone-*(trans)* or Benzalacetophenone $C_6H_5COCH{=}CHC_6H_5$	208.26	pa ye lf, pr, nd (peth)	345-8d, 208[15]	(i)59 (ii)57 (iii)49	1.0712[20/4]	.....	eth, bz, chl	B7[2], 2380
4849	Chalcone, 4,4-dimethyl $(4\text{-}CH_3C_6H_4)COCH{=}CH(C_6H_4CH_3\text{-}4)$	236.32	cr (MeOH)	.....	(27-9	.....	.....	al	B7[2], 441
4850	Chalcone, 3,3'-dinitroiro $(3\text{-}O_2NC_6H_4)COCH{=}CH(C_6H_4NO_2\text{-}3)$	298.25	pa ye nd (pal	.....	210-1	.....	.....	bz	B7[2], 2407
4851	Chalcone, 2-methoxy or 2-Anisylidene acetophenone $(2\text{-}CH_3OC_6H_4)CH{=}CHCOC_6H_5$	238.29	yesh nd (peth or eth-lig)	.....	64-5	.....	.....	al, eth, bz, chl	B8[2], 1456
4852	Chalcone, 3-methoxy $(3\text{-}CH_3OC_6H_4)CH{=}CHCOC_6H_5$	238.29	yesh pl or pr (MeOH)	247[14]	65	.....	.....	al, eth, ace, bz	B8[2], 1463
4853	Chalcone, 4-methoxy $(4\text{-}CH_3OC_6H_4)CH{=}CHCOC_6H_5$	238.29	ye nd (al)	187-8[15]	79	.....	.....	al, eth, chl, aa	B8[2], 1464
4854	Chalcone, 3,4-methylene dioxy or Piperonylidine acetophenone $(3,4\text{-}CH_2O_2)C_6H_3CH{=}CHCOC_6H_5$	252.27	ye nd (al)	.....	128	.....	.....	al, aa	B19[1], 1866
4855	Chalcone, 2-nitro $(2\text{-}O_2NC_6H_4)CH{=}CHCOC_6H_5$	253.26	pa bi nd (al)	.....	125	.....	.....	al, eth, aa	B7[2], 2399
4856	Chalcone, 2'-nitro $C_6H_5CH{=}CHCO(C_6H_4NO_2\text{-}2)$	253.26	nd (al)	.....	128-9	.....	.....	al, eth	B7[2], 2402
4857	Chalcone, 3-nitro $(3\text{-}O_2NC_6H_4)CH{=}CHCOC_6H_5$	253.26	ye nd (al or bz)	.....	145-6	.....	.....	al, bz, chl, aa	B7[2], 2400
4858	Chalcone, 4-nitro $(4\text{-}O_2NC_6H_4)CH{=}CHCOC_6H_5$	253.26	pa ye nd (al), pl (bz)	.....	164	.....	.....	al, chl	B7[2], 2401

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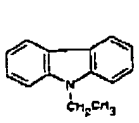
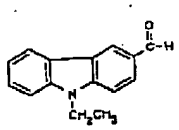
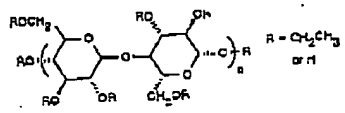
11,232-1 ★	**Ethyl caprylate, 99+ %** [*106-32-1*] (ethyl octanoate) $CH_3(CH_2)_6CO_2C_2H_5$ FW 172.27 mp -48 to -47° bp 208-208° *n*D 1.4170 d 0.878 Fp 167°F(75°C) *Beil.* 2,348 *Merck Index* 11,3736 *FT-NMR* 1(1),822A *FT-IR* 1(1),607C *SI* 104,A,6 *Safety* 2,1587B *R&S* 1(1),689L *RTECS#* RH0880000 *IRRITANT*	5g 100g 500g	9.10 19.90 69.80
	Ethyl carbamate, see U285-7, Urethane page 1520	25g	19.10
E1,650-3 ★	**Ethyl carbazate, 97%** [*4114-31-2*] $H_2NNHCO_2C_2H_5$ FW 104.11 mp 44-47° bp 108-110°/22mm Fp 187°F(86°C) *Beil.* 3,98 *Fieser* 1,360 *FT-NMR* 1(1),1266C *FT-IR* 1(1),776A *SI* 140,A,5 *Safety* 2,1567C *R&S* 1(1),909M *RTECS#* FE2545000 *FLAMMABLE SOLID IRRITANT*	5g 100g 500g	17.10 52.00 173.20
E1,660-0 ★	**9-Ethylcarbazole, 98%** [*86-28-2*] FW 195.27 mp 68-70° *Beil.* 20,436 *FT-NMR* 1(3),161A *FT-IR* 1(2),679D *SI* 364,A,7 *R&S* 1(2),2425C *RTECS#* FE6225700 *IRRITANT*	25g 100g	94.20 254.30
15,148-3	**9-Ethyl-3-carbazolecarboxaldehyde, 98%** [*7570-45-8*] FW 223.28 mp 85-87° *FT-NMR* 1(3),163C *FT-IR* 1(2),681A *SI* 384,E,6 *R&S* 1(2),2425M *IRRITANT*	5g 250g 500g	18.40 60.70 109.40
	Ethyl β-carboline-3-carboxylate, see 24,430-9, Ethyl 9*H*-pyrido[3,4-*b*]indole-3-carboxylate page 708		
	Ethyl carbonate, see D8155-1, Diethyl carbonate page 611		
20,067-0 ★	**Ethyl cellulose** [*9004-57-3*] *Merck Index* 11,3739 *FT-IR* 1(2),1178B *SI* 500,C,4 *Safety* 2,1588A *R&S* 1(2),3158M *RTECS#* FJ5950500 *IRRITANT* Powder. Ethoxyl content 46%. Softening point 155°C. Viscosity (5% solution in 60/40 toluene/ethanol) 100 cps. Density 1.17	5g 250g 500g	23.00 76.90 126.60
20,064-6 ★	**Ethyl cellulose** [*9004-57-3*] Powder. Ethoxyl content 48%. Softening point 155°C. Viscosity (5% solution in 80/20 toluene/ethanol) 4 cps	5g 250g 500g	17.10 56.30 93.90
20,068-9 ★	**Ethyl cellulose** [*9004-57-3*] Powder. Ethoxyl content 48%. Softening point 155°C. Viscosity (5% solution in 80/20 toluene/ethanol) 10 cps	5g 250g 500g	17.10 56.30 93.90
20,069-7 ★	**Ethyl cellulose** [*9004-57-3*] Powder. Ethoxyl content 48%. Softening point 156°C. Viscosity (5% solution in 80/20 toluene/ethanol) 22 cps	5g 250g 500g	17.10 56.30 93.90
43,383-7 ★	**Ethyl cellulose** [*9004-57-3*] Ethoxyl content 48 wt. %. Viscosity (5 wt. % solution in 80/20 toluene/ethanol) 46 cps. Tg 120-124°	5g 250g 500g	19.50 29.10 107.30
24,749-9 ★	**Ethyl cellulose** [*9004-57-3*] Powder. Ethoxyl content 48%. Softening point 155°C. Viscosity (5% solution in 80/20 toluene/ethanol) 100 cps. Density 1.13.	5g 250g 500g	17.10 56.30 93.90
20,065-4 ★	**Ethyl cellulose** [*9004-57-3*] Granules. Ethoxyl content 48%. Softening point 157°C. Viscosity (5% solution in 80/20 toluene/ethanol) 300 cps	5g 250g	23.00 70.30
18,102-1 ★	**Ethyl cellulose** [*9004-57-3*] Powder. Ethoxyl content 49%. Softening point 162°C. Viscosity (5% solution in 80/20 toluene/ethanol) 10 cps.	5g 250g 500g	23.00 75.90 126.60
20,066-2 ★	**Ethyl cellulose** [*9004-57-3*] Powder. Ethoxyl content 49%. Viscosity (5% solution in 80/20 toluene/ethanol) 100 cps.		
	Ethyl chloride, see Chloroethane	5g 25g	25.20 84.40
44,003-5 NEW	**Ethyl 4-(2-chloroacetamido)benzoate, 98%** [*26226-72-2*] $ClCH_2CONHC_6H_4CO_2C_2H_5$ FW 241.68 mp 110-114° *SI* 319,E,2	1g 10g 100g	12.60 69.60 27.30
44,543-6 NEW	**Ethyl 2-(2-chloroacetamido)-4-thiazoleacetate, 98%** [*19749-93-0*] FW 262.72 mp 146-148° *IRRITANT*		
24,071-0 ★	**Ethyl chloroacetate, 99+ %** [*105-39-5*] $ClCH_2CO_2C_2H_5$ FW 122.55 mp -26° bp 143° *n*D 1.4210 Fp 150°F(65°C) *Beil.* 2,197 *Merck Index* 11,3741 *FT-NMR* 1(1),1008A *FT-IR* 1(1),650D *SI* 113,A,1 *Safety* 2,1588B *R&S* 1(1),735A *RTECS#* AF8110000 *HIGHLY TOXIC LACHRYMATOR*		



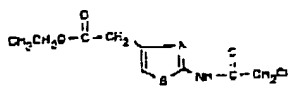
E1,660-0



15,148-3



18,102-1



44,543-6